Some thermal transport properties of the FPU model with quadratic pinning

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Abstract

Thermal transport properties of the FPU β model with a quadratic pinning term are investigated for various couplings and temperatures. In particular, the size dependence of the thermal conductivity, $\kappa \propto L^{\alpha}$, is studied. α agrees with that of the FPU β model (with no pinning) at high temperatures but decreases at low temperatures. This crossover behavior occurs at a temperature depending on the strength of the quadratic pinning.

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Physics of non-equilibrium is of importance to a broad range of issues in science. Consequently, non-equilibrium physics has been studied for a long time, yet a number of basic problems remain. Thermal transport in one dimensional systems, while seemingly simple, has been an area of intriguing active research for a long time[1]. The FPU model is one of the most classic models in studies of non-equilibrium physics and a natural model defined on a lattice, so that it has been studied from various points of view[1]. By virtue of being well studied, many of its properties in the non-equilibrium steady state are known and has been quite useful as a guide in studying non-equilibrium physics in various models at finite temperatures. One of the key intriguing properties of the model is the lack of bulk behavior in thermal transport. Specifically, the thermal conductivity of the model is known to behave as $\kappa \propto L^\alpha$, where L is the size of the system and α ranges from $1/3$ to $2/5$[1, 2, 3, 4, 5, 6, 7].

In this work, we study thermal properties of a model which generalizes the so called FPU β model by including a quadratic pinning term and study its properties, from first principles. The Hamiltonian of the theory is

$$H' = \sum_{k=1}^{L} \left[\frac{p_k'^2}{2m} + m\omega^2 \frac{(q_{k+1}' - q_k')^2}{2} + \frac{\mu' q_k'^2}{2} + \beta \frac{(q_{k+1}' - q_k')^4}{4} \right] \tag{1}$$

We study the statistical mechanical properties related to thermal transport and analyze how the behavior changes with the the physical parameters in the theory. FPU model combined with the quartic and quadratic pinning potentials and with randomness have been studied recently[8, 9, 10].

Let us explain why we find this model interesting: The FPU model does not have bulk behavior, as mentioned above. This can be attributed to the translational symmetry of the theory[1, 11] and is seen in a range of similar models. Any pinning term, such as the one we introduce in (1) destroys this symmetry, so that the model may achieve bulk behavior. However, if we ignore the quartic FPU interaction, the model described by (1) is none other than a harmonic model whose exact solutions are known and do not display sensible bulk behavior[12, 13]. So by combining these models, we have a situation wherein neither model has bulk behavior, yet the combined model might, which we investigate. Also, there are arguments as to why the size dependence of the thermal conductivity is universal in theories with translational symmetry[2, 4, 5]. As we remove this symmetry, we expect that the size dependence will not be the same so that we have a model in which the size dependence can change naturally with the parameters of the theory. An objective here is to obtain insight

into the thermal properties of the model by studying how α changes with the physical parameters. Furthermore, the model is a fairly simple one generalizing the well studied FPU model. As such, knowing the properties of the model globally in parameter space, we hope, will enhance our understanding of the thermal transport properties of similar theories.

Let us first reduce the model to its simplest form without any loss in generality. Using the rescalings in q_k, p_k and time, we obtain the following form of the Hamiltonian, similarly to the FPU model[3].

$$H = \sum_{k=1}^{L} \left[\frac{p_k^2}{2} + \frac{(\nabla q)_k^2}{2} + \frac{\mu q_k^2}{2} + \frac{(\nabla q)_k^4}{4} \right] \tag{2}$$

Here, the variables are related as $q' = \omega\sqrt{m/\beta}\,q$, $p' = \omega^2\sqrt{m^3/\beta}\,p$, $\mu' = m\omega^2\mu$, $H' = (m^2\omega^4/\beta)H$. We also adopted the notation $\nabla q_k \equiv q_{k+1} - q_k$ for convenience. The temperature in the two formulations are related as $T = \beta T'/(m^2\omega^4)$, and T is effectively the strength of the FPU coupling, similarly to the FPU model and the ϕ^4 theory[3, 14]. The model has a coupling constant, μ, the strength of the quadratic pinning. As we can see from the reparametrizations, the quadratic pinning becomes more important for low temperatures. The size L of the system is a parameter of the model which enters intrinsically into transport properties, if the model does not have bulk behavior. We choose to fix the quartic coupling and vary T, since it seems more natural to fix the system and vary the temperature, but one may equivalently fix T and vary the coupling, due to the above rescaling degrees of freedom.

We now investigate the thermal transport properties of this system by studying its non-equilibrium steady states. The energy flow in the system is defined locally as $J_k = -p_k\nabla q_k(1 + \nabla q_k^2)$. The system at finite temperature has three parameters μ, L, T and we try to elucidate the physics behind the dependence on these parameters, similarly to the case of $\mu = 0$ in [3]. Let us briefly describe how the thermal conductivity, κ, is computed: Non-equilibrium steady states are numerically constructed for a given set of μ, L and T using thermostats generalizing the Nosé–Hoover thermostats, at the boundaries[15, 16]. In this work, we thermostatted two sites at each end of the system at temperatures (T_1^0, T_2^0). Away from these thermostatted boundary points, the behavior of the system is governed dynamically by the Hamiltonian (2), including the boundary temperature jumps. One crucial point is that the thermostats we employ are known to be able thermalize the harmonic oscillator chain[16], which the classic Nosé-Hoover thermostats can not[15, 17]. This is relevant

here since as we vary the parameters, the system in some cases will approach the harmonic model. The classical equations of motion were integrated numerically using the Runge–Kutta method with time steps of 0.002 to 0.02. The physical results were checked to be stable against variations in the size of the time step. 10^7 to few times 10^9 data were averaged to obtain the physics results. The system sizes used varied from $L = 36$ to $L = 4000$. Fixed boundary conditions are used throughout. The standard ideal gas thermometer, $T = \langle p_k^2 \rangle$, was used to measure the temperature locally.

Thermal conductivity is obtained from Fourier's Law

$$J = -\kappa \nabla T \tag{3}$$

where J is the heat current. To obtain κ, multiple non-equilibrium states are constructed around the same average temperature T to confirm that Fourier's law is valid and also to reduce error. This also allows us to check that the we are not too far away from equilibrium and that the linear response still holds. This is performed for fixed values of μ and L. Examples of thermal profiles in non-equilibrium steady states are shown in Fig. 1.

In order to obtain κ reliably, the following two points need to be taken care of. Traditionally, one often obtains α through the behavior of the heat current J for fixed boundary conditions as $JL \sim L^{\alpha_J}$. However, in general, temperature jumps arise at the boundaries, as seen in Fig. 1, and this needs to be taken into account[18]. Due to the jumps, the gradient is not $(T_2^0 - T_1^0)/L$, but smaller. Since the jumps are proportional to the boundary temperature gradients[19, 20], they will be smaller for larger systems when the boundary conditions are fixed. Consequently, there is a tendency for $\alpha_J \geq \alpha$ to hold. A way to avoid this is to measure the thermal gradient inside the system, away from the boundaries, as we shall do so here. This is particularly important when the system has parameters such that its is close to the harmonic limit and has large boundary jumps. The occurrence of large jumps is consistent with the exact analytic results known for the harmonic chains, whose thermal profiles consist essentially only of boundary jumps[12, 13]. Some profiles with their linear fits for deriving the gradient are shown in Fig. 1, which illustrate this behavior. Another issue that needs to be addressed is the validity of the linear response theory. If we stray too far from equilibrium, J will deviate appreciably from linear response theory. Here, we check that the linear relation holds and that we keep the gradients to be not too large for each parameter set. A priori, there is no rule as to whether J has to be larger or smaller than

the linear response prediction, but in the FPU model and the ϕ^4 theory, $|J|$ is smaller than what is expected from $\kappa\nabla T$[21]. If the boundary temperature differences are fixed while varying L, ∇T is larger for smaller systems so that they are further from equilibrium. This effect can lead to an underestimation of κ for smaller systems, which in turn can also lead an overestimation of α. The problem can be avoided by checking Fourier's law (3) or using the knowledge of how large the deviation from the linear response theory is. While it will not play an important role here, curvature in the profiles can also affect the extraction of κ in general.
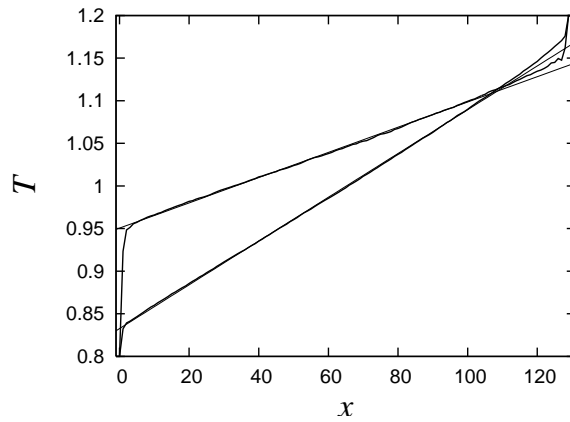

FIG. 1: Temperature profiles with $\mu = 1$ for $(T_1^0, T_2^0) = (0.8, 1.2), (0.08, 0.12)$. Temperature has been rescaled as $2T/(T_1^0 + T_2^0)$. Jumps are larger for the latter boundary conditions. Linear fits to the profiles away from the boundaries are also shown but they fit the profile so well that they can be seen only close to the boundaries.

The dependence of the conductivity with various values of μ are shown in Fig. 2. Let us try to understand the physics behind the main characteristics of the behavior of κ. In general, for low and high temperatures, κ increases, as in the FPU β model ($\mu = 0$). At high temperatures, κ for different μ tends to converge since the quartic coupling dominates the theory and the effect of the quadratic pinning is relatively small. At low temperatures, the theory approaches the harmonic limit and κ diverges. Differences due to μ are significant in this regime.

By obtaining κ for various values of L with respect to a given set of μ, T, the size dependence α may be obtained for the particular set of parameters, μ, T. The dependence of α on T for various values of μ are shown in Fig. 3. The behavior of α can be summarized
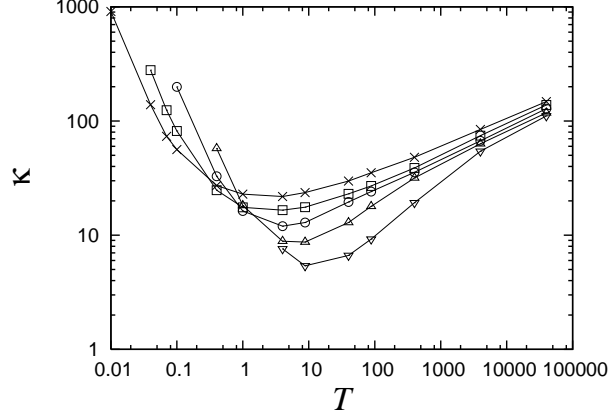
FIG. 2: Temperature dependence of κ with $L = 132$, for $\mu = 0$ ($\times$), $\mu = 1$ ($\square$), $\mu = 4$ ($\bigcirc$), $\mu = 10$ ($\triangle$) and $\mu = 30$ ($\triangledown$). The results for the same value of μ have been joined for clarity.
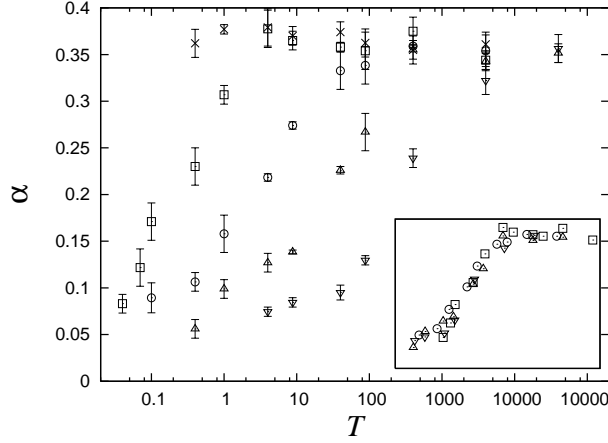

FIG. 3: α vs. T for $\mu = 0$ ($\times$), $\mu = 1$ ($\square$), $\mu = 4$ ($\bigcirc$), $\mu = 10$ ($\triangle$) and $\mu = 30$ ($\triangledown$). Inset shows the same points (for $\mu \neq 0$) with the rescaled temperature T/μ^2 (see text).

as follows: At higher temperatures, α converges to one value and it is consistent with the previous literature for the FPU β model [1, 2, 3, 4, 5, 6, 7]. When $\mu \neq 0$, at lower T, the dependence α decreases with T. The crossover behavior to decreasing α occurs at larger T for larger μ. This is natural since the effect of the pinning term is greater for larger μ so that the crossover occurs at a higher temperature.

The decrease in α can be understood as the effect of pinning, with the tendency towards bulk behavior. This change in α occurs at low T since this is the region where the quadratic term is dominant and the quartic FPU coupling is weak. The validity of the argument can be confirmed from the dominant term in the potential, which indeed changes as we vary the

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temperature. This crossover behavior can be investigated in equilibrium and an example of this is seen in Fig. 4. The time averages of the terms in the potential, μq_k^2, $(\nabla q)_k^2$ and $(\nabla q)_k^4$ will equal T, if the term by itself completely dominates the potential, from the virial argument. We note here that in the equilibrium system, the expectation values of μq_k^2, $(\nabla q)_k^2$ and $(\nabla q)_k^4$ do not vary inside the system. The above understanding of the crossover allows us to compute roughly the crossover temperature, which we denote as T_c.

$$q^4 \sim T \ (T \gg 1), \qquad \mu q^2 \sim T \ (T \ll 1) \quad \Rightarrow \quad T_c \sim \mu^2 \tag{4}$$

The estimate is consistent with the crossover temperatures seen in Fig. 3. The picture also suggests that a more general scaling with the rescaled temperature T/μ^2 might apply. The behavior of α with respect to this rescaled temperature is shown in the inset and the scaling works well in practice. We do not have a rigorous argument for this scaling behavior and it is worth further study. While there is visibly different behavior below and above this "crossover temperature", we expect this not to be a sharp transition. For $T \lesssim T_c$ and α not too small, the behavior seems to be reasonably well described by

$$\alpha = \alpha_0 + \nu \ln \frac{T}{T_c}, \qquad \nu = 0.055(5) \tag{5}$$

Here, we denoted the common value of α high temperature constant as α_0. If we naively extrapolate this behavior to low temperatures, $\alpha = 0$ is reached at a finite temperature, $T_c \exp(-\alpha_0/\nu)$, but we cannot reliably extrapolate to this limit. Paradoxically, numerical determination of α is exceedingly difficult for small α values, where we naively expect the system to have bulk behavior. This is because in the model described by (2), small α values occur close to the harmonic limit where the gradients become small and are difficult to compute reliably. This difficulty precludes us from definitely predicting what happens in the limit $\alpha \to 0$. Several scenarios are possible: The model might reach $\alpha = 0$ at finite T. In this case, if κ is finite, the system has bulk behavior. It is also possible that the behavior for small T is not described by the log behavior (5) and that κ diverges in the $\alpha \to 0$ limit, which is also the $T \to 0$ limit and this limit coincides with the harmonic model. In this case, the model can, in some sense, be arbitrarily close to having bulk behavior yet does not achieve it for finite values of the physical parameters. We consider this last possibility to be the most likely. It can be noticed that the crossover temperature for the FPU β model ($\mu = 0$) is $T_c = 0$ so that it is never reached, if the above scaling is applied. However, the model is quite different from $\mu \neq 0$ cases so that it should be studied separately.
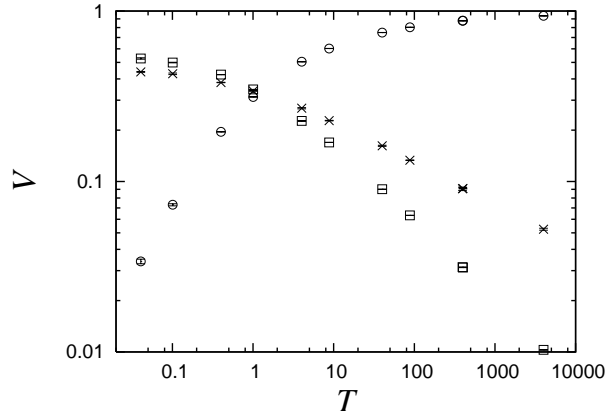
FIG. 4: Temperature dependence of $\langle \mu q^2 \rangle / T$ ($\times$), $\langle (\nabla q)^2 \rangle / T$ ($\square$) and $\langle (\nabla q)^4 \rangle / T$ ($\bigcirc$) for $\mu = 1$.

The behavior of the system as it becomes closer to the harmonic limit perhaps needs to be explained. In the harmonic limit, one might expect $\kappa \propto L$ behavior with α being one, so that α should rather increase than decrease when T is smaller. This behavior is suggested by the exact analytic solutions for the harmonic models[12, 13]; in these solutions, for fixed boundary thermostat temperatures, $T^0_{1,2}$, J is independent of L. Naively, the gradient varies as $(T^0_2 - T^0_1)/L$ so that κ should be proportional to L. However, this argument completely ignores the boundary effects. With boundary jumps, which are dynamical, the gradient is not directly related to the boundary thermostat temperatures and $\alpha_J = 1 \gtrless \alpha$. In fact, in the harmonic case, the gradient is zero inside the system so that κ effectively diverges even for a finite size system, which is consistent with the behavior of κ for small T in our results, as in Fig. 2. Given the divergence of κ, there is no analytic prediction for α in the harmonic limit. One property of the harmonic model is the independence of J with respect to L for fixed boundary thermostat temperatures. We find that the dependence of J on L does indeed become weaker at lower temperatures. The dynamics of the interior adjusts the gradient so that the conductivity has a weaker dependence on L.

In this work, we computed thermal transport properties of the FPU β model with a quadratic pinning potential for various values of the pinning potential, temperature and system size. We have analyzed the dependence of the conductivity on the physical parameters of the theory and have obtained an understanding of them. Had we included the quartic potential, the theory should have bulk behavior in some parameter region[8, 9, 10]. However, in the model discussed, none of the couplings by themselves lead to bulk behavior of the

system and the total system does not reach the bulk limit. At low temperatures, where the quartic coupling is effectively weak, the quadratic pinning term becomes more important. This reduces α (in $\kappa \propto L^\alpha$) so that the transport behavior is closer to bulk behavior. However, the system governed by quadratic terms is harmonic and the conductivity, at the same time, approaches divergent behavior.

The size dependence, α, varies with parameters of the theory. We have used this power α in this study but it is worth noting that a priori, there is no rigorous proof that κ should behave homogeneously as a power of L, even though we find that the behavior applies quite well in practice. Some questions remain: In particular, the precise limiting behavior of the theory can not be obtained numerically, so that a rigorous theoretical reasoning is quite desirable, particularly close to the harmonic limit. To this end, one might envisage an application of perturbation theory around the harmonic theory to the FPU quartic coupling, similar in spirit to the perturbation theory applied to the quartic pinning coupling [22]. From this perspective, one can view the theory with the quadratic pinning in the FPU theory as the extrapolation between the harmonic model with a continuous variation of the size dependence of the thermal conductivity.

[1] J. Ford, Phys. Rep. 213 (1992) 271; S. Lepri, R. Livi, A. Politi, Phys. Rep. 377 (2003) 1

[2] S. Lepri, R. Livi, A. Politi, Phys. Rev. Lett. 78, 1896 (1997); Europhys. Lett. 43, 271 (1998).

[3] K. Aoki, D. Kusnezov, Phys. Rev. Lett. 86 (2001) 4029.

[4] O. Narayan, S. Ramaswamy, Phys. Rev. Lett. 89, 200601 (2002).

[5] S. Lepri, R. Livi, A. Politi, Phys. Rev. E 68, 067102 (2003).

[6] A. Pereverzev, Phys. Rev. E 68, 056124 (2003).

[7] T. Mai, A. Dhar, O. Narayan, Phys. Rev. Lett. 98 184301 (2007).

[8] L. Wang, B. Li, Phys. Rev. B 74, 134204 (2006).

[9] A. Dhar, J.L. Lebowitz, `arXiv:0708.4171`.

[10] N. Li, B. Li, Phys. Rev. 76, 011108 (2007).

[11] T. Prosen, D. Campbell, Phys. Rev. Lett. 84, 2857 (2000).

[12] Z. Rieder, J.L. Lebowitz, E. Lieb, J. Math. Phys. 8, 1073 (1967).

[13] H. Nakazawa, Suppl. Prog. Theo. Phys. 45, 231 (1970)

[14] K. Aoki, D. Kusnezov, Ann. Phys. 295, 50 (2002); Phys. Lett. B477, 348 (2000).

[15] S. Nosé, J. Chem. Phys. 81, 511 (1984); Mol. Phys. 52, 255 (1984); W. G. Hoover, Phys. Rev. A 31,1695 (1985).

[16] D. Kusnezov, A. Bulgac, W. Bauer, Ann. Phys. 204 (1990) 155

[17] H.A. Posch, Wm.G. Hoover, F.J. Vesely, Phys. Rev. A 33, 4253 (1986).

[18] T. Hatano, Phys. Rev. E59 R1 (1999).

[19] E. M. Lifshits, L.P. Pitaevskii, Physical Kinetics, (Pergamon Press, New York, 1981).

[20] K. Aoki, D. Kusnezov, Phys. Lett. A265 (2000) 250

[21] K. Aoki, D. Kusnezov, *Phys. Lett.* **A309** (2003) 377; K. Aoki, Phys. Lett. A368 77, (2007)

[22] R. Lefevere and A. Schenkel, J. Stat. Mech.2006, L02001 (2006).